Progress in Surface Science

An International Review Journal

EDITOR: Professor Sydney G. Davison

AUTHOR AND SUBJECT INDEX

Volume 26, 1987

PERGAMON PRESS

New York / Oxford / Toronto
Paris / Frankfurt / Sydney

Progress in Surface Science

EDITOR:
PROF. SYDNEY G. DAVISON

Applied Mathematics Department
University of Waterloo
Waterloo, Ontario
Canada N2L 3G1

MANAGING EDITOR:
PROF. W.K. LIU

Physics Department
University of Waterloo
Waterloo, Ontario
Canada N2L 3G1

ADVISORY BOARD

I. BARTOS
Academy of Sciences
Prague, Czechoslovakia

B.E. CONWAY
University of Ottawa
Ontario, Canada

A.S.G. CURTIS
University of Glasgow,
Scotland

A.W. CZANDERNA
Solar Energy Research Institute
Golden, Colorado, U.S.A.

D.D. ELEY
University of Nottingham,
England

P.J. ESTRUP
Brown University
Providence, Rhode Island, U.S.A.

J.W. GADZUK
National Bureau of Standards
Gaithersburgh, Maryland, U.S.A.

V.E. HENRICH
Yale University
New Haven, Connecticut, U.S.A.

N.I. IONOV
Academy of Sciences
Leningrad, U.S.S.R.

J. KOUTECKY
Freie Universitat
Berlin, F.R. Germany

R.M. LATANISION
Massachusetts Institute of Technology
Cambridge, Massachusetts, U.S.A.

J.D. LEVINE
Texas Instruments
Dallas, Texas, U.S.A.

A.A. MARADUDIN
University of California
Irvine, California, U.S.A.

S.R. MORRISON
Simon Fraser University
Burnaby, Canada

K. MULLER
University of Erlangen-Nurnberg
West Germany

R. PARSONS
University of Southampton, England

J.B. PENDRY
Imperial College
London, England

S.T. PICRAUX
Sandia National Laboratory
Albuquerque, New Mexico, U.S.A.

T.N. RHODIN
Cornell University
Ithaca, New York, U.S.A.

S. SUGANO
University of Tokyo, Japan

H. TI TIEN
Michigan State University
East Lansing, Michigan, U.S.A.

L. WEISS
Roswell Park Memorial Institute
Buffalo, New York, U.S.A.

R.F. WILLIS
Pennsylvania State University
University Park, Pennsylvania, U.S.A.

Publishing, Subscription and Advertising Offices: Pergamon Press, Inc., Fairview Park, Elmsford, New York 10523, U.S.A. and Pergamon Press plc, Headington Hill Hall, Oxford OX3 0BW, England.

Published Monthly: 3 volumes per year, 4 issues per volume. Annual institutional subscription rate (1990): DM850.00; Two-year institutional rate (1990/91): DM1615.00; Personal subscription rate for those whose library subscribes at the regular rate: DM213.00. Prices are subject to change without notice. Notify 8 weeks in advance of address change with a copy of the subscription mailing label. Microform subscriptions: Information available upon request.

Copyright © 1990 Pergamon Press plc.

The paper used in this publication meets the minimum requirements of American National Standard for Information Sciences — Permanence of Paper for Printed Library Materials, ANSI Z39.48-1984

It is a condition of publication that manuscripts submitted to this journal have not been published and will not be simultaneoulsy submitted or published elsewhere. By submitting a manuscript, the authors agree that the copyright for their article is transferred to the publisher, if and when the article is accepted for publication. The copyright covers exlusive rights to reproduce and distribute the article, including reprints, photographic reproductions, microform or any other reproductions of similar nature and translations. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, electrostatic, magnetic tape, mechanical, photocopying, recording or otherwise, without permission in writing from the copyright holder.

Photocopying information for users in the U.S.A.: The Item-Fee Code for this publication indicates that authorization to photocopy items for internal or personal use is granted by the copyright holder for libraries and other users registered with the Copyright Clearance Center (CCC) Transactional Reporting Service provided the stated fee for copying beyond that permitted by Section 107 or 108 of the United States Copyright Law is paid. The appropriate remittance of $0.50 per page is paid directly to the Copyright Clearance Center Inc., 27 Congress Street, Salem, MA 01970.

Permission for other use. The copyright owner's consent does not extend to copying for general distribution, for promotion, for creating new works, or for resale. Specific written permission must be obtained from the publisher for such copying. Please contact the Subsidiary Rights Manager, at either Pergamon Press, Inc. or Pergamon Press plc.

The Item-Fee Code for this publication is: 0079-6816/89 $0.00 + .50

AUTHOR INDEX

Abrahamson, A.A. 46
Adams, J.E. 99
Adams, W. 174
Albuquerque, E.L. 116
Allen, M.C. 198
Amitani, K. 219
Amos, A.T. 46, 61, 74
Anderson, A.B. 198
Anderson, P.W. 17, 46, 85, 174
Appelbaum, J.A. 133, 174
Arias, J. 45
Ashcroft, N.W. 163
Auerbach, D.J. 99
Avouris, Ph. 85

Babiker, M. 116
Backx, C. 99
Baetzold, R. 219
Baetzold, R.C. 219
Bagus, P.S. 199
Baker, B.G. 212
Bange, K. 99
Baquero, R. 133
Baraff, G.A. 133, 142
Bartós, I. 116
Bastard, G. 116
Bauer, R.S. 133
Bauschlicher, C.W., Jr. 199
Beck, T.L. 163
Becker, G.E. 85
Bedford, K.L. 174
Benndorf, C. 199
Bennemann, K.H. 180
Benziger, J. 198
Benziger, J.B. 199
Bernasek, S.L. 199
Bernholz, J. 142
Berry, R.S. 163
Beveridge, D.L. 198, 219
Bhaduri, R.K. 163
Bhasu, V.C.J. 46, 61, 74
Biczó, G. 142
Biloen, P. 99
Blandin, A. 17, 46
Blint, R.J. 174
Bloomfield, L.A. 163
Bloss, W. 46, 61
Blyholder, G. 198
Bogomolov, V.N. 163
Bohr, A. 163
Bönig, L. 17
Bozco, F. 45
Brako, R. 17, 46, 61
Brenig, W. 46
Brivio, G.P. 17
Brogensma, H.H. 46
Brown, W.L. 163
Buck, T.M. 46
Bykhovskii, V.K. 61

Cade, P.E. 219
Callaway, J. 142, 180
Camley, R.E. 116
Campbell, C.T. 198
Car, R. 163
Catlow, C.R.A. 219
Chadi, D.J. 132
Chang, L.L. 116
Chen, M.Y. 180
Chen, R.S. 142
Chiaradia, P. 133
Chou, M.Y. 163
Chudnovskii, F.A. 163
Cini, M. 46
Cleland, A. 163
Clemenger, K. 163, 180
Clementi, E. 198, 219
Cohen, M.L. 163, 180
Colligon, J.S. 45
Cosma, G. 85
Coulson, C.A. 198
Cox, D.M. 180
Cunningham, S.L. 133
Curl, R.F. 163

Das, G. 199
Das, T.P. 219
Davison, S.G. 46, 61, 74, 115, 116
de Brouckere, G. 198
de Dominicis, C. 17
de Groot, C.P.M. 99
de Heer, W.A. 163, 180

de Zwart, S.T. 85
Del Re, G. 142
Dendramis, R.J. 198
Demkov, Yu.N. 61
Deutsch, P.W. 174
Dhar, S. 180
Djafari-Rouhani, B. 115, 116
Dobryzynski, L. 115, 116
Donelon, J.J. 85
Dovesi, R. 143
Dow, J.D. 132
Duparc, O.H. 115
Dwyer, D.J. 199
Dy, K.S. 116

Eachus, R.S. 219
Easa, S.I. 46
Eastman, D.E. 85
Efrima, S. 61
Erickson, R.L. 46
Esaki, L. 116, 132

Falicov, L.M. 116, 212
Fantucci, P. 180, 198
Fine, J. 74
Flores, F. 133
Freed, K.F. 61
Freeman, A.J. 198, 212
Freeman, R.R. 163
Freiser, B.S. 198
Fu, C.L. 198

Gadzuk, J.W. 46, 99
Garciá-Molinar, F. 116, 132, 133
Garrison, B.J. 99
Gauyacq, J.P. 74
Geerlings, J.J.C. 45, 74
Gehring, J. 45, 46
Gentry, W.R. 99
George, T.F. 46
Gerber, R.B. 99
Gilbert, T.L. 174
Gislason, E.A. 99
Gland, J.L. 199
Goddard, W.A. III 61, 174
Goodenough, J.B. 198
Gouverneur, L. 142
Granneman, E.H.A. 45, 74
Grant, R.W. 133
Grimley, T. 142
Grimley, T.B. 17, 46, 61, 74
Grimm, D. 85
Gumhalter, B. 85
Gunnarsson, O. 17, 85, 212
Guse, M.P. 174
Gutschik, V.P. 99

Hagstrum, H.D. 45, 85
Hamann, D.R. 133, 174
Hanawa, T. 61
Handy, N.C. 99
Harding, J.H. 219
Harker, A.H. 219
Harrison, W.A. 133
Hay, P.J. 174
Hayes, W. 219
Hayns, M.R. 219
Head, J. 198
Heath, J.R. 163
Heer, J. 132
Heiland, W. 46, 99
Heine, V. 180
Heller, E.J. 99
Helmbrecht, U. 163
Hermann, J. 45, 46
Hermann, K. 199
Hikkelsen, J.C. 133
Himpsel, F.J. 85
Hjalmarson, H.P. 132
Hjelmberg, H. 212
Holloway, S. 99
Hone, D. 61
Hone, D.W. 17, 46
Hood, E. 61
Horvatić, B. 85
Howard, W.E. 132
Hunt, W.J. 174

Ichinokawa, T. 163
Idiodi, J.O.A. 115
Imke, U. 99
Inglesfield, J.E. 61
Ishii, Y. 163
Itoh, N. 219

Jedrzejek, C. 61
Jellinek, J. 163
Jena, P. 163
Jensen, J.H.D. 163
Jette, A.M. 219
Jiang, H.X. 116
Joannopoulos, J.D. 116
Johanson, G.J. 180
Johnson, E.B. 212
Johnson, K.H. 180
Jugnet, Y. 85

Kaldor, A. 180
Kamemitsu, Y. 219
Kant, A. 198
Karikorpi, M. 99
Kasauski, R.V. 174
Katakuse, I. 163

Katnani, A.D. 133
Kawai, H. 61
Kawai, R. 46, 61
Kawakami, N. 61
Kempter, V. 45, 46
Kertesz, M. 142
Klein, D.L. 174
Kleinman, L. 212
Kleyn, A.W. 99
Klushin, N.A. 163
Knight, W.D. 163, 180
Koch, E.E. 85
Kohda, K. 219
Koster, G.F. 132, 142
Koutecký, J. 115, 142, 163, 174, 180, 198
Krakaver, H. 212
Kraus, J. 46
Kraut, E.A. 133
Kruger, B. 199
Kübler, J. 180
Kung, A.Y.S. 219
Kunz, A.B. 174, 219

Ladik, J. 142, 143
Landau, L. 61
Landgren, G. 85
Lane, K.R. 198
Lang, N.D. 46, 212
Langreth, D.C. 163
Lee, D.H. 116
Lee, H.W. 46
Lee, J. 99
Lee, K. 180
Leroy, G. 142
Leung, C.H. 219
Lichten, W. 46
Liebich, B.W. 219
Lin, J.H. 99
Lin, J.Y. 116
Lipari, N. 142
Liu, W.-K. 85
Liu, Y. 163
Lopez-Sancho, J.M. 116, 132
Lopez-Sancho, M.P. 116, 132
Los, J. 45, 74, 99
Lovrić, D. 85
Lu, J.P. 199
Lundqvist, B.I. 46, 212
Lyon, S.B. 219

Madey, T.E. 74, 99
Madhaven, P.V. 212
Madix, R.J. 99, 198, 199
Maire, G.I.C. 212
Makoshi, K. 17, 46, 74
Makoshi, S. 61
Manneback, C. 99
Manninen, M. 163
Maradudin, A.A. 116
Marion, J.B. 99
Marshall, R.F. 174
Martin, R.L. 212
Martin, R.M. 45
Marx, A. 85
Masri, P. 115, 116
McGirr, M.B. 180
Mendes, E.E. 116
Messmer, R.P. 198
Metiu, H. 45, 61
Meyer, M.G. 163
Mickish, D.J. 174
Miller, W.H. 99
Miyahara, J. 219
Miyoshi, E. 212
Modinos, A. 45, 46
Moon, D.W. 199
Moon, K.A. 198
Moore, C.E. 212
Morar, J.F. 85
Mott, N.F. 46
Mottelson, B.R. 163
Moyer, C.A. 61
Muda, Y. 61
Mukerjee, S. 180
Munõz, A. 133
Munõz, M.C. 132
Muscat, J.-P. 85

Nagvi, K.R. 99
Nakamura, T. 212
Neff, S.H. 46
Nekin, C.J. 199
Neumann, J. 99
Newns, D.M. 17, 46, 61, 85
Newton, M.D. 212
Nicollin, D. 219
Nieber, B. 199
Nieto, M.M. 99
Nikitin, E.E. 61
Nishina, Y. 163
Nørskov, J.K. 46, 212
Nourtier, A. 17, 46
Nozières, P. 17

Oden, C. 85
Ohnishi, A. 163
Ohnishi, S. 163
O'Brien, S.C. 163
Okiji, A. 61
Okuneva, N.M. 163
Orvek, K. 61

Osherov, V.I. 61
Otto, P. 142, 143
Ovchinnikova, M.Ya. 61
Overbosch, E.G. 45, 74

Pacchioni, G. 163, 198
Pakkanen, T.A. 212
Pandaripande. V/R/ 163
Pantelides, S.T. 133, 142
Parrinello, M. 163
Perdew, J.P. 163
Pfnür, H.E. 99
Pieper, S.C. 163
Pippard, A.B. 99
Pisani, C. 143
Placehnova, E.L. 163
Poelsema, B. 85
Pogrebnoi, V.I. 163
Pollack, R.A. 85
Pollmann, J. 133
Pople, J.A. 198, 219
Puszkarski, H. 115

Raghavachari, K. 163
Raimondi, D.L. 198, 219
Rao, B.K. 163
Rapp, D. 99
Rasser, B. 45, 74
Ray, N.K. 198
Rettner, C.T. 99
Robinson, M.T. 46
Rodnik, R. 74
Rodriguez, J. 198
Rohlfing, C.M. 212
Rohlfing, E.A. 180
Rosenzweig, L.N. 115
Ross, C.K. 163
Rovetti, C. 143
Robio, J. 116, 132
Ruette, F. 198
Rusch, T.W. 46

Saito, S. 163
Sakaki, H. 116
Sallans, L. 198
Sanchez-Dehesa, J. 133
Sang, H.W., Jr. 133
Sass, J.K. 99
Satoko, C. 163
Saul, P. 219
Saunders, W.A. 163, 180
Sawada, S. 163
Schall, H. 46
Scheer, M.D. 74
Schlüter, M. 142
Schlüter, M.A. 163
Schmidling, D. 198
Schneir, J. 85
Schönhammer, K. 17, 46, 85
Schubert, S. 99
Schwartz, R.N. 99
Sebastian, K.L. 46, 61, 74
Seel, M. 142
Shima, N. 61
Shindo, S. 46, 61
Shionoya, S. 219
Simmons, L.M. 99
Slater, J.C. 132, 142
Smalley, R.E. 163
Smith, D.P. 45, 46
Smith, J.R. 174
Snowden, K.J. 99
Sokčević, D. 85
Somorjai, G.A. 212
Song, K.S. 219
Spratlin, T. 116
Squires, R.R. 198
Šroubek, Z. 45, 46
Stechel, E.B. 99
Stoneham, A.M. 219
Strutinsky, V.M. 163
Stueckelberg, E.C.G. 61
Sugano, S. 163
Sulston, K.W. 46, 61, 74, 115

Taglauer, E. 46
Takahashi, K. 219
Tamura, A. 163, 173
Tasker, P.W. 219
Tatewaki, H. 212
Tenner, A.D. 45, 74
Tersoff, J. 212
Tilley, D.R. 116
Tittle, F.K. 163
Tolk, N.H. 46
Tománek, D. 163, 180
Tomonaga, S. 17
Trevor, D.J. 180
Tsuchiya, M. 116
Tsukada, M. 61
Tsuneyuki, S. 61
Tully, J.C. 46, 61

Ueba, H. 116
Upton, T.H. 61, 174

Vail, J.M. 219
van Amersfoort, P.W. 74
van Wuunik, J.N.M. 45, 46, 61
Van Zee, R. 198
Varga, P. 99

Vasile, M.J. 46
Velasco, V.R. 116, 132, 133
Vogl, P. 132

Wachters, A.J.H. 212
Walch, S.P. 199
Waldenstrom, S. 99
Waldrop, J.R. 133
Wandelt, K. 85
Welle, B. 46
Weltner, W., Jr. 198
Wheeler, D.A. 180
Whetten, R.L. 180
White, C.W. 46
Whitten, J.L. 212
Williams, A.R. 46, 212
Williams, P. 46
Wimmer, E. 198, 212
Woodruff, D.P. 46
Wu, Shi-Yu 116

Yamada, K. 17
Yares, J.T., Jr. 45
Yndurain, F. 116
Yoshimori, A. 17, 46, 61, 74
Yoshino, J. 116
Yosida, K. 17
Yu, M.L. 46

Zabolitzky, J.G. 163
Zartner, A. 46
Zavadil, J. 46
Zdetsis, A.P. 174
Zener, C. 61
Zhang, Q.-L. 163
Zlatić, V. 85
Zunger, A. 163
Zurcher, P. 133

SUBJECT INDEX

Adatoms, effect on atom-surface scattering process 67-74
Adsorbates. See also Resonance occupation effects on adsobates.
  electron spectroscopies and valence resonance relaxation 82-85
  intra-adsorbate electronic transitions 77-79
  polarization properties, valence resonance occupation effect on 79-81
  resonance occupation effects on 75-85
Adsorption
  diatomic energies and analysis of 181-198
  effects of adsorbed atoms 63-74
    ionization probability calculation, unrestricted H-F formalism 65-67
    Na-Na/W(110) system and 67-74
  effects on charge transfer, atom-surface scattering 63-74
  ionization probability and 65-73
  Na-Na/W(110) system and 67-74
Atom-surface scattering. See also Resonance charge transfer, atom-surface scattering.
  adsorption effects on resonance charge transfer 63-74
  Auger transitions and 23
  classical mechanics 22
  ion neutralization and 23-24
  noble-ion-backscattering 22-23
  resonance charge transfer in 19-45

Band effect, electron transfer probability 49-52
  Anderson Hamiltonian, time-dependent 49
  energy-level crossing 51-52
  resonance tunnelling and 50-51, 52-53
  time-developing operator and 49-50

Charge transfer. See Resonance charge transfer, atomic scattering.
Chemisorption studies, embedded cluster methods 166-174
Cluster models. See Embedded cluster models.
Clusters. See also specific categories.
  embedded clusters 166-174
  metal clusters, atomic and electronic structure 149-157
  microclusters, atomic and electronic structure 147-162
  semi-conductor clusters, Si_6 and Si_{10} 157-161
  transition-metal clusters 178-180
CNDO (complete neglect of differential overlap) method and parameters 214-215. See also Defects, electron and hole, in halide alkali earths.
Coulomb repulsion, intra-atomic
  excited states, scattered atoms, formation of 39-40
  Hartree-Fock method and 36-37
  time-dependent coupled-cluster approach 37-39

Defect, surface and chemisorption studies 166-174. See also Embedded cluster methods, surface defect and chemisorption studies.
Defects, electron and hole, in halide alkaline earths
  cluster models, BaFBr 215-218
    band structure 217
    defect centers, properties of 217-218
    density of unpaired electron on defect centers 217
    one-electron energies 215-216, 218
    valence band edge energies and 215-216, 218
  CNDO method and parameter selection 214-215, 219

Diatomic energies, analysis of adsorption and coadsorption and 181-198
adsorption and reaction of CO 181-183
cluster model 182
molecular orbital model 181, 182, 188-189, 191, 193, 195, 197
Fe_{12}-CO 4-fold 190-192, 193
Fe_{12}-CO on-top 189-191, 193
Fe_{12}-H results 186-189
Fe-H results 185-186
H-Fe_{12}-CO 192-195
H-Fe_{12} 4-fold 194, 196, 197
MINDO/SR calculational procedures
atom cluster and 183
Fe atomic and bond parameters 183-184

Electronic energy levels, semiconductor clusters 159-160
Electronic friction, metals and metal surfaces
energy distribution function 3, 12-17
energy transfer rate 7-12
model, one-electron states 3-5
time-dependent one-electron states 3, 5-7
Electronic states, Ni(001) surface atom 201-212
calculations
configuration interaction (CI) wave functions formulation 205
molecular orbital 203-204
self-consistent field (SCF) 202-203
charge transfer, sp- to d-band 202
CI calculations and results
SCF-MO basis, d^9 configuration 207-210
vs. interaction of states calculations, valence electronic energies 207, 208
wave functions formulation 205
d-occupation and 202
interaction of states 208, 210-211
results
CI calculations 205, 207
SCF energies, d occupancies of states 205-206
unrestricted SCF (USCF), relaxation effects and 205, 206-207
spin states 212
Electronic transitions, adsorbate
intra-adsorbate 77-79, 80
valence resonances and 76-77
Electrons
defects of, halide alkaline earths 213-219
model of 3-5
one-electron states, time-dependent 3, 5-7
Electron transfer, adparticle and surface, in surface dynamical processes 47-60
band effect on dynamical charge exchange probability 49-53
coupling with medium effect 57-60
boson system and 59, 60
phonon-mediated system 59-60
time-dependent Hartree approximation and 57-58, 59
field-induced desorption and charge exchange process 53-57
quantum mechanical treatment vs. simplified models 48
Embedded cluster methods, surface defect and chemisorption studies 166-174
applications of 167
approach assumptions 173
energy band methodologies 166, 173
Green's function approaches 168, 173
lattice periodicity and 167-168
perturbative approach 173
finite cluster methods 166-167
general formalism 168-172
canonical transformation 170
Hartree-Fock approximation 169
local orbital problem and 172
many body Hamiltonian, Born-Oppenheimer approximation 168-169
zero order problem and 170-171
strong interactions method 167-168
supercell method 168
Empirical tight-binding Hamiltonian. See also Semi-conductor interfaces, nonideal, tight-binding model.
eigenvalues for fitting procedure 118
surface Green functions matching 118-119
Energy. See also specific categories.
cohesive energy, transition metal clusters 176-177, 178, 179

(Energy, cont.)
diatomic energies, adsorption and co-adsorption analysis 181-198
Energy distribution function, friction in metals 3, 12-17
boson approximation and Debye-Waller factor 14-16
perturbation, diagonal and non-diagonal 12-13
perturbation excitation 12
Energy exchange, classical trajectory model and 91-92
Energy transfer processes, surface and substrate 2
Energy transfer rate, electron friction in metals 7-12
classical result 11
integral calculation of 8-9
time-dependent dissipation rate 10
velocity dependence dissipation rate 10-11
ETB. See Empirical tight-binding Hamiltonian.

Field-induced desorption (FID), charge exchange process
adiabatic and nonadiabatic surface of system 53
barrier height determination 54-55, 57
reaction rate determination 55-57
Friction. See Electronic friction.
Fusion research, charge exchange processes and 20

Harmonic oscillator. See also Surface reaction dynamics, harmonic oscillator.
classical trajectory model and 89-93
quantum molecules and 93-98
Hartree approximation, time-dependent (TDH) 57-58, 59
Hartree-Fock (H-F) approximation, finite cluster methods and 166
Hartree-Fock (H-F) formalism
ionization probability and unrestricted 65-67
Na-Na/W(110) systen and 69-74
Hartree-Fock method
intra-atomic Coulomb repulsion and 36-37
one-electron H-F method 214, 219

Interaction of states, Ni(001) surface atom, 208, 210-211
Interface response theory, discrete superlattices
continuous response function and 115
general theory 104-133
general equation for 108
interface response operator $\overleftrightarrow{A}$ 107-108
matrix elements of response function $\overleftrightarrow{g}$ 108-113
N-layered supperlattice definition 104-105
physical properties of N-layered superlattices 112-113
response functions 105-107
simple models, exact solutions 113-114
Interfaces, semi-conductor. See Semiconductor interfaces, nonideal, tight-binding model.
Ion-survival probability, oscillatory 40-45
Ionization-level occupancy as function of time, atom-surface scattering charge transfer and 68-69
Ionization probability
calculation, unrestricted H-F formalism and 65-67
charge transfer in atom-surface scattering and 69-73
as function of incident atom kinetic energy 69-71
versus work function 71-73
H-F formalism, unrestricted 65-67

Na-Na/W(110) system and 69-74

Jellium model, spherical, alkali metal clusters and 150, 151

Lattices
ionic, defects in and CNDO method 214
superlattices, discrete 103-115

Microclusters, atomic and electronic structure 147-162
computers and computation technique advances 148
dynamical properties of 161-162
electronic shell structure, alkali and noble metal clusters 148
metal clusters 149-157
cluster ions, positive and negative, mass spectra 149
liquid drop model 150, 155-156

(Microclusters, metal...,cont.)
magic number in sodium clusters 149
multiplets formation, ground state stabilization 152
nonspherical perturbation 153-155
shell correction, deformed metal clusters 155-157
shell effects in alkali metal clusters 155-157
spherical jellium model, alkali metal clusters 150, 151
spin polarization and stabilization 151
semi-conductor clusters, Si_6 and Si_{10} 157-161
electron densities 160-161
electronic energy levels 159-160
reconstruction, atomic 157-159
MINDO/SR 183-184. See also Diatomic energies, calculational procedures.
Molecules
molecule-surface scattering, generic 89
quantum, harmonic oscillator and surface reaction dynamics 93-98

One-electron Hartree-Fock method 214, 219
One-electron properties, adsorbate/surface, perturbative approaches to 173. See Embedded cluster methods, surface defect and chemisorption studies.
One-electron theory
model, one-electron states 3-5
time-dependent one-electron states 3, 5-7
Oscillatory ion-survival probability 40-45

Perturbation
diagonal and nondiagonal 12-13
nonspherical, microclusters and 153-155
time-depdendent diagonal and nondiagonal 2, 3-5

Quasi-one-dimensional chains, ab-initio self-consistent field (SCF) theory 137-142
extension of formalism and procedure 142
(Quasi-one-dimensional chains, cont.)
formulation of method
ab-initio SCF LCAO 137
Dyson equation and 138-139
Green matrices and 138
numerical procedure 139-141

Relaxation effects and structural stability, transition-metal clusters 179
Relaxation mechanisms, intra-adsorbate electronic transitions 77-78
Resonance charge transfer in atom-scattering
adsorption effects of adsorbed atoms 63-74
ionization probability calculation, unrestricted H-F formalism 65-67
Na-Na/W(110) system and 67-74
Coulomb repulsion, intra-atomic 36
excited states, scattered atoms, formation of 39-40
H-F method 36-37
time-dependent coupled-cluster approach 37-39
one-electron theory 24-36
atom-surface system, time-evolved state of 30-33
charge state, sputtered atoms 27-29
low-temperature nearly-adiabatic limit 26-27
parallel motion effect 35-36
reflection, Na from W(110) 33-35
semi-classical approximation 29-30
time-dependent A-N Hamiltonian 24-26
oscillatory ion-survival probability 40-45
Resonance occupation effects on adsorbate, dynamical electronic properties and 75-85
adsorbate electronic transitions, valence resonances and 76-77
electron spectroscopy, adsorbates and valence resonance relaxation 82-85
intra-adsorbate electronic transitions 77-79, 80
classification of 77
relaxation mechanisms of excitations 77-78
valence resonance occupation effect, polarization of adsorbates 79-81

Self-consistent field theory, ab-initio, quasi-one-dimensional (1D) chain interfaces 135-142. See also Quasi-one-dimensional (1D) chain interfaces.
applications of 136-137
Green's matrix formalism and 136
Koster-Slater method, ab-initio, H-F self-consisitent field 136
linear bomcination of atomic orbitals, ab-initio fully self-consistent method 135
Semi-conductor interfaces, nonideal, tight-binding model 117-132
empirical tight-binding calculations 118-119
practical application, Ge-GaAs(110) heterojunctions
ideal (100) interface Ge-Ga case band structure 124-125, 131
ideal Ge-As case 126, 130
ideal interface model 124
local changes of density of states 129-130
stoichiometrically mixed model 124, 127-129, 131
valence band and 125
problem formulations, SGFM formulae and 119-123
atomic layers, definition of corresponding 119
ideal vs. nonideal interfaces 119-120
surface Green function matching and 118-119
Sputtering and charge transfer 20, 21
Superlattices, discrete
continuous response function theories of 115
N-layered superlattices 105
bulk response function, each submaterial K 105-106
physical properties of 112-113
reference response function $\overleftrightarrow{g}$ of 106-107
slab K , one homogeneous material 104
slab N of different homogeneous material 105
superlattices, polytype 105
Surface Green function matching formalism (SGFM), semi-conductor interafces and 118, 119-123, 131-132
Surface reaction dynamics, harmonic oscillator and 87-98
(Surface reaction...,cont.)
classical trajectory model 89-93
energy exchange, translational to vibrational 92-93
molecule-surface scattering, generic 89
potential energy surfaces and 89-91
trajectories for vibrationally cold O_2 molecule 91-92
harmonic oscillator, molecule-surface reactions and 88-89
quantum molecules 93-98
classical vs. quantum harmonic oscillator 93
Frank-Condon picture, vibrational state distribution 95, 98
Poisson distribution of excited states 93-95, 98
quadratic potential propagation 95
vibrational state distribution 90, 95-96, 98

TDH. See Time-dependent Hartree approximation.
Time-dependent Hartree (TDH) approximation, charge exchange process and 57-58, 59
Transition-metal clusters 175-180
bond length and 177, 178
cohesive energy and 176-177, 178, 179
magnetic order and 180
relaxation effects and structural stability 179

Valence resonance occupation effect, adsorbate polarizability and 79-81
Valence resonance relaxation, electron spectroscopy of adsorbates 82-85

XANES (X-ray adsorption near edge structure). See Adsorbates, electron spectroscopy.
XPS (X-ray photoemission spectroscopy). See Adsorbates, electron spectroscopy.